

Topological Quantum Chemistry and its applications in materials search

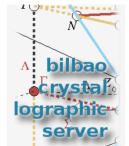
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6.29.2019 漂阳



Acknowledge

- The Bilbao Crystallographic Server (BCS):
<http://www.cryst.ehu.es/>
- Collaborators: B. Andrei Bernevig (PU); Barry and Jennifer (PCTS, Princeton); Luis, Mois and Maia (Bilbao, Spain); Claudia (Max-Planck Institute)
- Ref: "Topological quantum chemistry", Nature, 547 (2017)



Bilbao Crystallographic Server
in forthcoming schools and workshops

News:

- New Article in *Acta Cryst. A* 05/2019:
Gallego et al. "Automatic calculation of symmetry-adapted tensors in magnetic and non-magnetic materials: a new tool of the Bilbao Crystallographic Server."
Acta Cryst. (2019). A75

bilbao crystallographic server



Quick access to some tables

Space Groups

Plane Groups

Layer Groups

Rod Groups

Frieze Groups

2D Point Groups

Collaborators



Barry Bradlyn
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Mois Aroyo (EHU)



Andrei Bernevig
(Princeton)

Outline

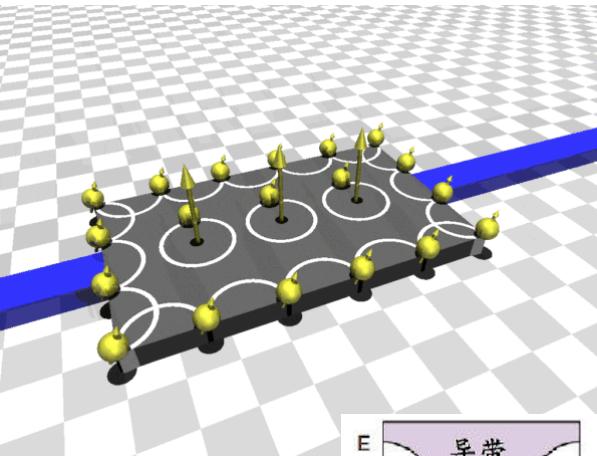
- Brief introduction to topological states
- Topological Quantum Chemistry (TQC)
- Applications in materials search

Outline

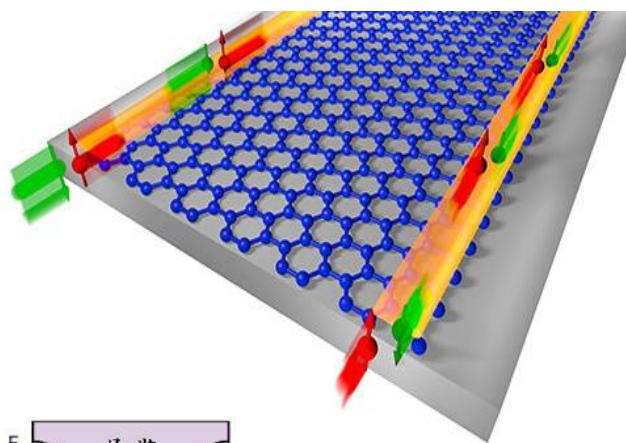
- Brief introduction to topological states
- Topological Quantum Chemistry (TQC)
- Applications in materials search

Introduction

QHE(量子霍尔效应)



QSHE(量子自旋霍尔)

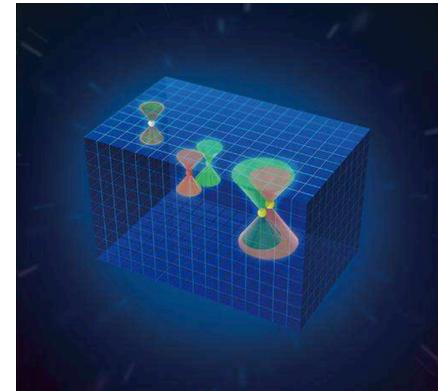
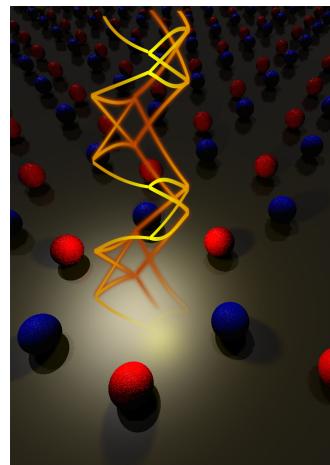
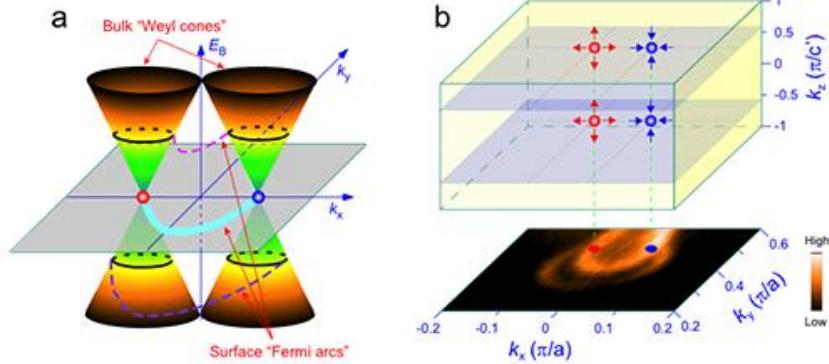
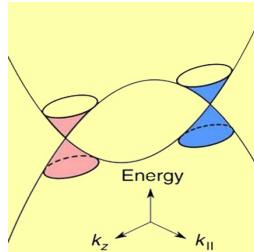


3DTI (拓扑绝缘体)



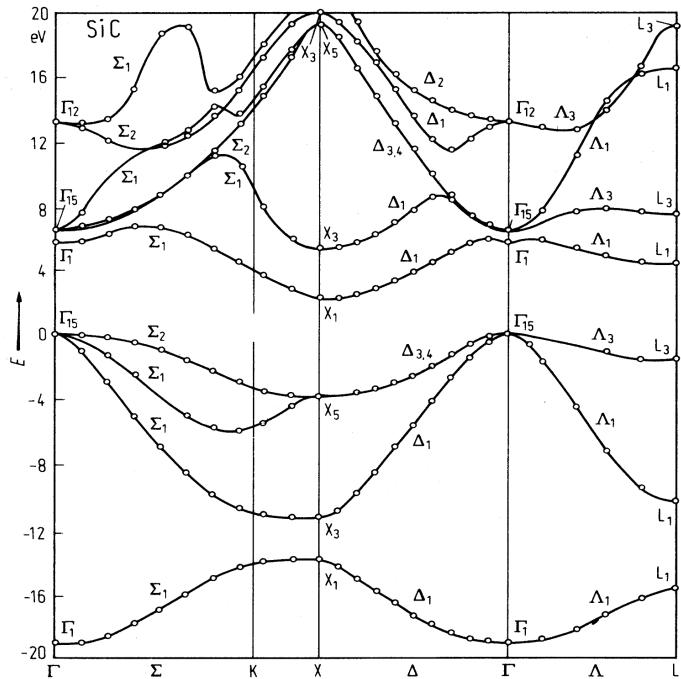
Other topological states

- Dirac semimetals: Na₃Bi and Cd₃As₂
- Weyl semimetal: TaAs
- Hourglass fermion: KHgSb.
- Spin-1 fermion : CoSi



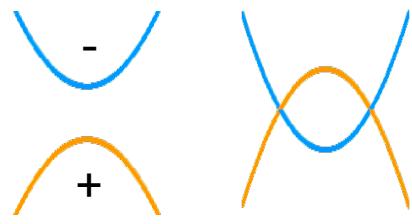
Band inversion

Band structure

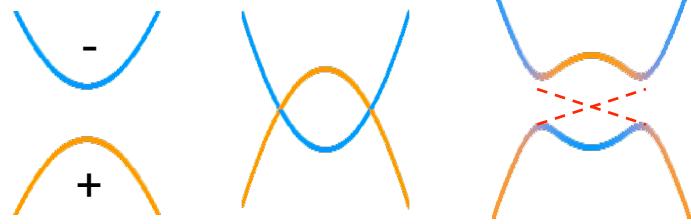


Spin-orbital coupling (自旋轨道耦合)

拓扑平庸态
普通绝缘体

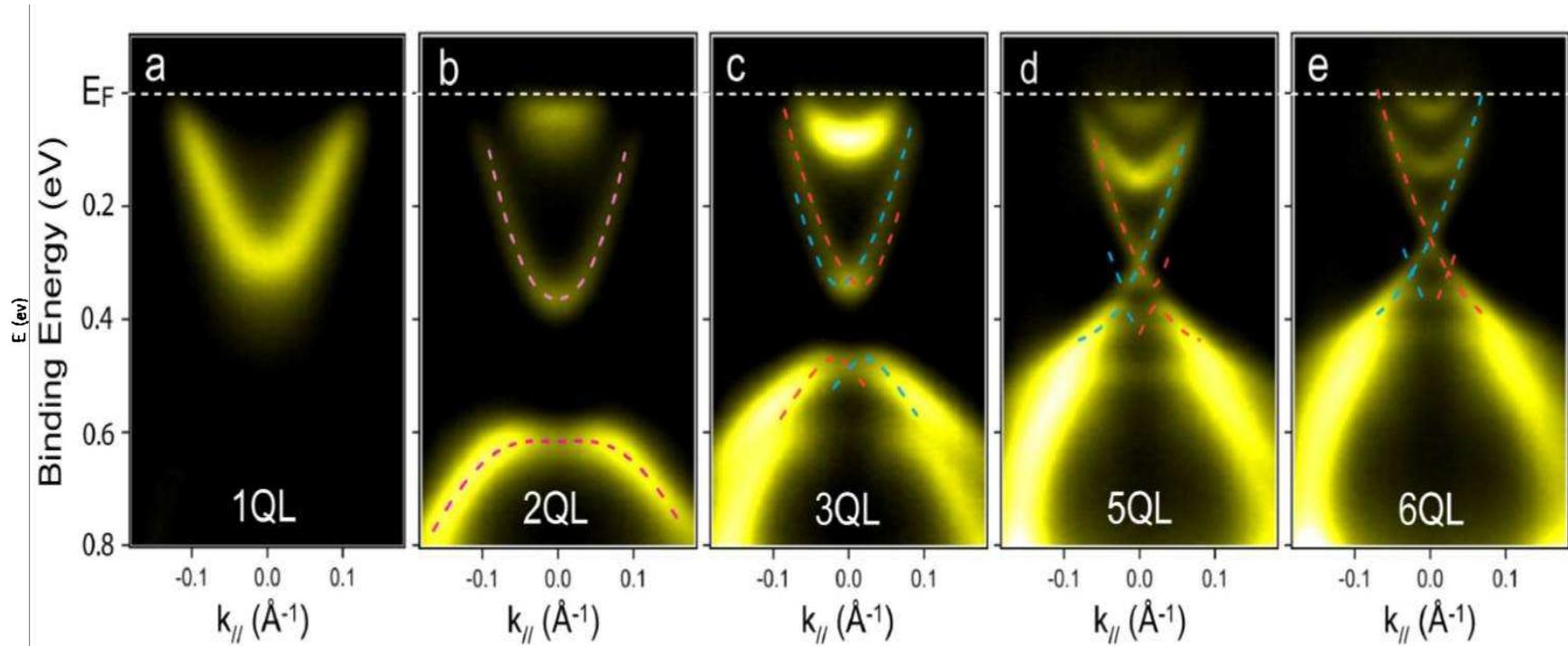


拓扑非平庸态
拓扑绝缘体



Gamma point

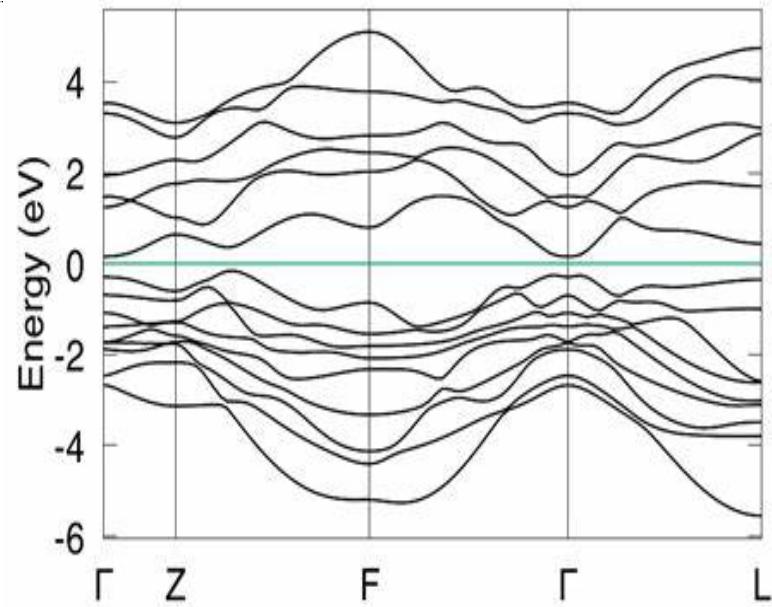
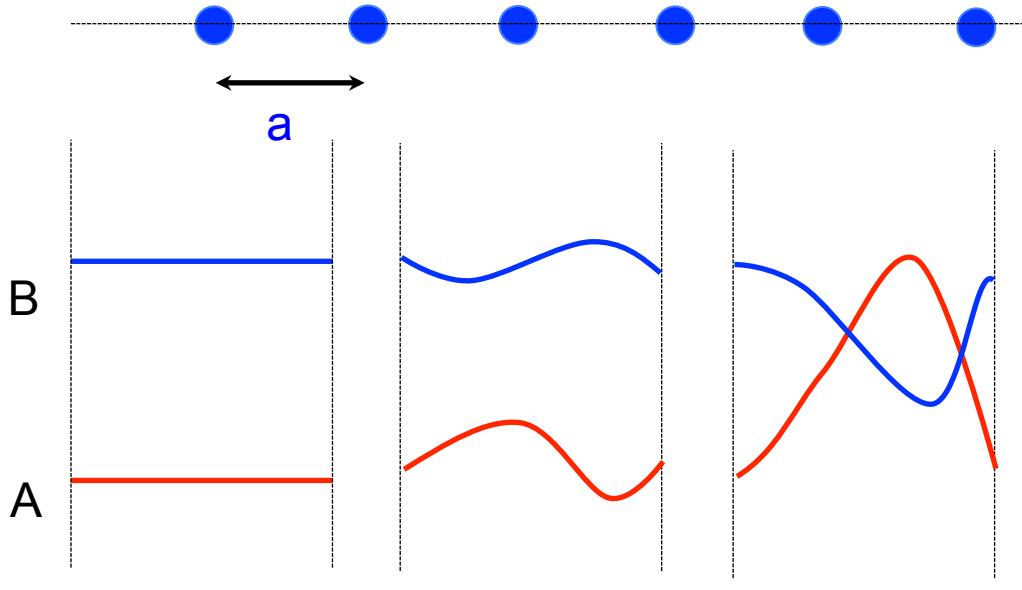
Band inversion



Outline

- Brief introduction to topological states
- Topological Quantum Chemistry (TQC)
- Applications in materials search

Band structure in 3D crystals



- Phase transition can only happen at the gap-closing point
- Topological band structures should not be atomic-limit band structures.

Space group

- Symmetry operator: $g = \{ R | t \}$
Space group G is a set of g operators.
- Translation symmetries $T: \{ la_1 + ma_2 + na_3 \}$
 k , normal subgroup
- Symmorphic v.s. Non-symmorphic space groups
 $G = \{ T, g_2 T, g_3 T, \dots \}$

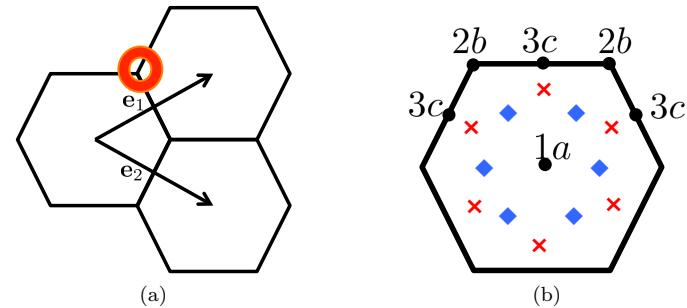
TQC

- (Maximal) Wyckoff position (q)
- Site symmetry (G_q)
- (Elementary) band representation

Wyckoff position (WP)

- Formalization: **site-symmetry** – each position \mathbf{q}
- Ex (6mm) : ($G_{\mathbf{q}}$: isomorphic to a point group)

$$G_{(\frac{2}{3}, \frac{1}{3})} = \langle \{C_{3z}|10\}, \{m_{1\bar{1}}|1\bar{1}\} \rangle$$



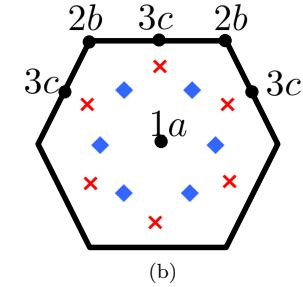
- Orbitals at \mathbf{q} transform in representation $G_{\mathbf{q}}$.

Wyckoff position (WP)

- Formalization: **site-symmetry** – each position \mathbf{q}
Wyckoff Positions of Group $P6mm$ (No. 183)

-

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
12	f	1	(x,y,z) $(-y,x-y,z)$ $(-x+y,-x,z)$ $(-x,-y,z)$ $(y,-x+y,z)$ $(x-y,x,z)$ $(-y,-x,z)$ $(-x+y,y,z)$ $(x,x-y,z)$ (y,x,z) $(x-y,-y,z)$ $(-x,-x+y,z)$
6	e	.m.	$(x,-x,z)$ $(x,2x,z)$ $(-2x,-x,z)$ $(-x,x,z)$ $(-x,-2x,z)$ $(2x,x,z)$
6	d	..m	$(x,0,z)$ $(0,x,z)$ $(-x,-x,z)$ $(-x,0,z)$ $(0,-x,z)$ (x,x,z)
3	c	2mm	$(1/2,0,z)$ $(0,1/2,z)$ $(1/2,1/2,z)$
2	b	3m.	$(1/3,2/3,z)$ $(2/3,1/3,z)$
1	a	6mm	$(0,0,z)$



Band representation

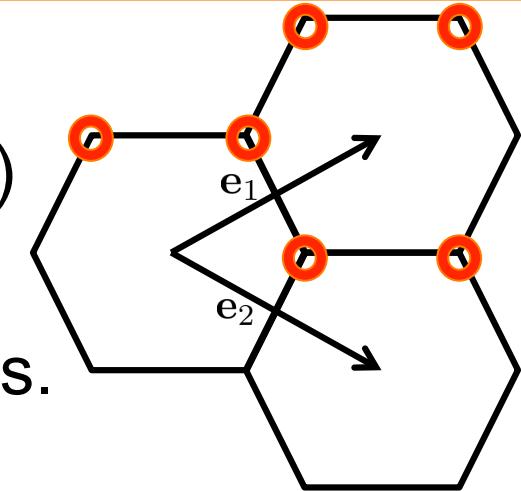
- Wyckoff position (\mathbf{q})
- Representations ($G\mathbf{q}$) (atomic Ins.)

$$a_{i\alpha}(\mathbf{k}, \mathbf{r}) = \sum_{\mu} e^{i\mathbf{k}\cdot\mathbf{t}_{\mu}} W_{i\alpha}(\mathbf{r} - \mathbf{t}_{\mu}),$$

- Matrix representation for all k-points.

$$(\rho_G(h)a)_{i\alpha}(\mathbf{k}, \mathbf{r}) = e^{-i(h\mathbf{k})\cdot\mathbf{R}_{\beta\alpha}} \sum_{i'=1}^{n_{\mathbf{q}}} \rho_{i'i}(g_{\beta}^{-1}\{E\} - \mathbf{R}_{\beta\alpha}) h g_{\alpha} a_{i'\beta}(h\mathbf{k}, \mathbf{r})$$

with $\mathbf{R}_{\beta\alpha} = h g_{\alpha} \mathbf{q} - g_{\beta} \mathbf{q}$

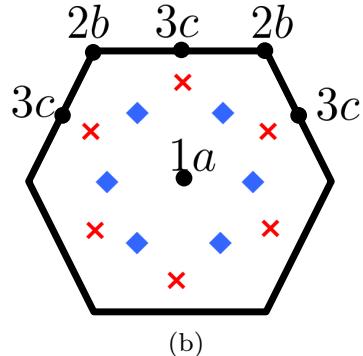


- Ref: Supplementary Information of "Topological quantum chemistry", Nature, 547 (2017)

Elementary band representation

- **Maximal** Wyckoff position q;
- **Irreducible** representations (irreps) at q (G_q)

Wyckoff Positions of Group $P6mm$ (No. 183)



Multiplicity	Wyckoff letter	Site symmetry	Coordinates
12	f	1	(x,y,z) $(-y,x-y,z)$ $(-x+y,-x,z)$ $(-x,-y,z)$ $(y,-x+y,z)$ $(x-y,x,z)$ $(-y,-x,z)$ $(-x+y,y,z)$ $(x,x-y,z)$ (y,x,z) $(x-y,-y,z)$ $(-x,-x+y,z)$
6	e	.m.	$(x,-x,z)$ $(x,2x,z)$ $(-2x,-x,z)$ $(-x,x,z)$ $(-x,-2x,z)$ $(2x,x,z)$
6	d	..m	$(x,0,z)$ $(0,x,z)$ $(-x,-x,z)$ $(-x,0,z)$ $(0,-x,z)$ (x,x,z)
3	c	2mm	$(1/2,0,z)$ $(0,1/2,z)$ $(1/2,1/2,z)$
2	b	3m.	$(1/3,2/3,z)$ $(2/3,1/3,z)$
1	a	6mm	$(0,0,z)$

Elementary band representation (EBR)

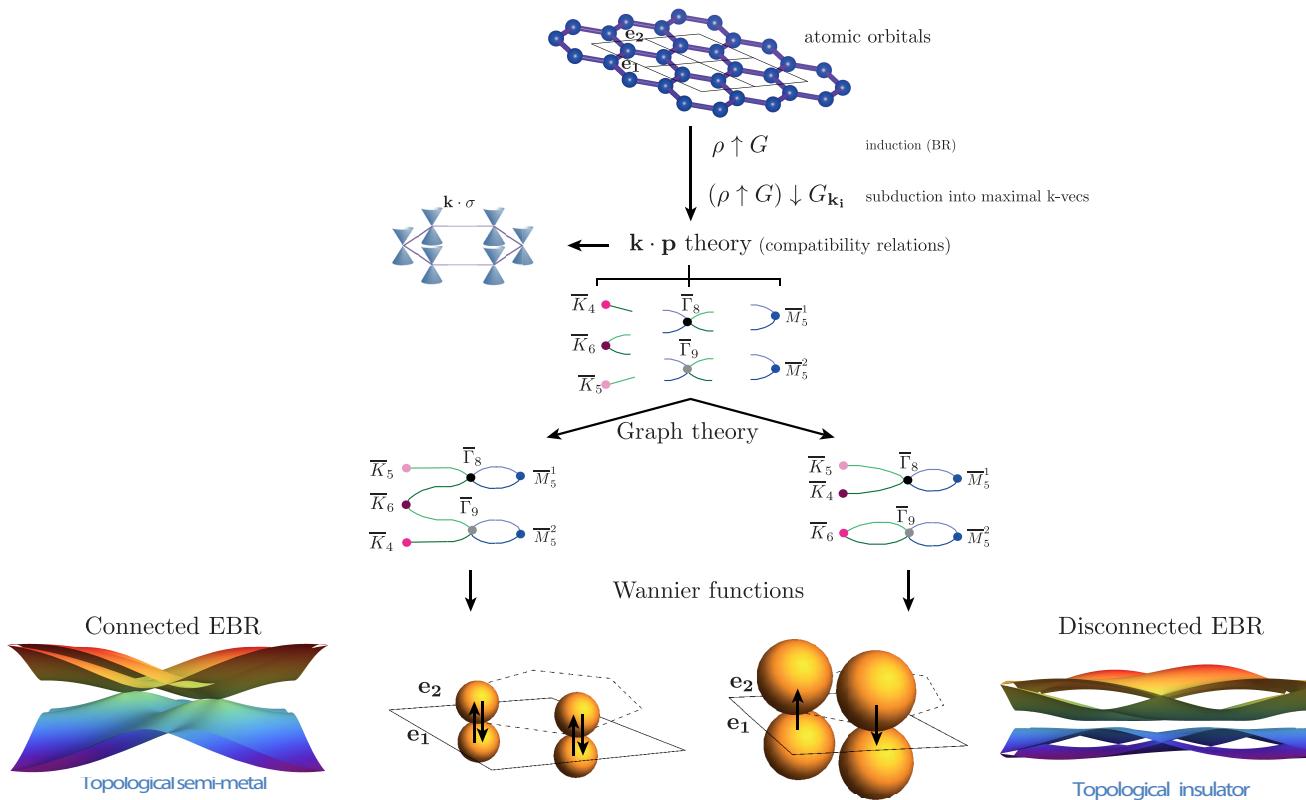
- Irreps at all **high-symmetry** k-points.

Wyckoff pos.	1a(6mm)	1a(6mm)	1a(6mm)	1a(6mm)	1a(6mm)	1a(6mm)	2b(3m)
Band-Rep.	A ₁ ↑G(1)	A ₂ ↑G(1)	B ₁ ↑G(1)	B ₂ ↑G(1)	E ₁ ↑G(2)	E ₂ ↑G(2)	A ₁ ↑G(2)
Decomposable Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable
A:(0,0,1/2)	A ₁ (1)	A ₂ (1)	A ₄ (1)	A ₃ (1)	A ₆ (2)	A ₅ (2)	A ₁ (1) ⊕ A ₄ (1)
Γ:(0,0,0)	Γ ₁ (1)	Γ ₂ (1)	Γ ₄ (1)	Γ ₃ (1)	Γ ₆ (2)	Γ ₅ (2)	Γ ₁ (1) ⊕ Γ ₄ (1)
H:(1/3,1/3,1/2)	H ₁ (1)	H ₂ (1)	H ₂ (1)	H ₁ (1)	H ₃ (2)	H ₃ (2)	H ₃ (2)
K:(1/3,1/3,0)	K ₁ (1)	K ₂ (1)	K ₂ (1)	K ₁ (1)	K ₃ (2)	K ₃ (2)	K ₃ (2)
L:(1/2,0,1/2)	L ₁ (1)	L ₂ (1)	L ₄ (1)	L ₃ (1)	L ₃ (1) ⊕ L ₄ (1)	L ₁ (1) ⊕ L ₂ (1)	L ₁ (1) ⊕ L ₄ (1)
M:(1/2,0,0)	M ₁ (1)	M ₂ (1)	M ₄ (1)	M ₃ (1)	M ₃ (1) ⊕ M ₄ (1)	M ₁ (1) ⊕ M ₂ (1)	M ₁ (1) ⊕ M ₄ (1)

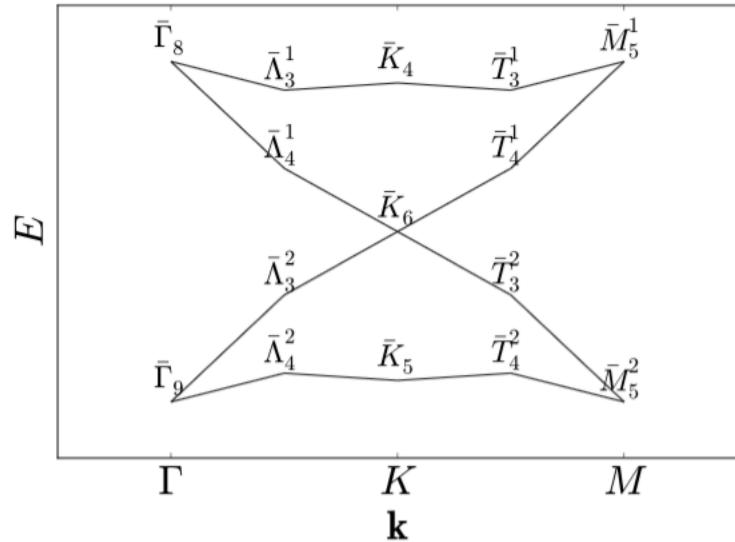
- Compatibility relations (on the BCS)

The maximal k -vectors are the set of high-symmetry points for which the determination of band characters implies their knowledge everywhere in the Brillouin zone.

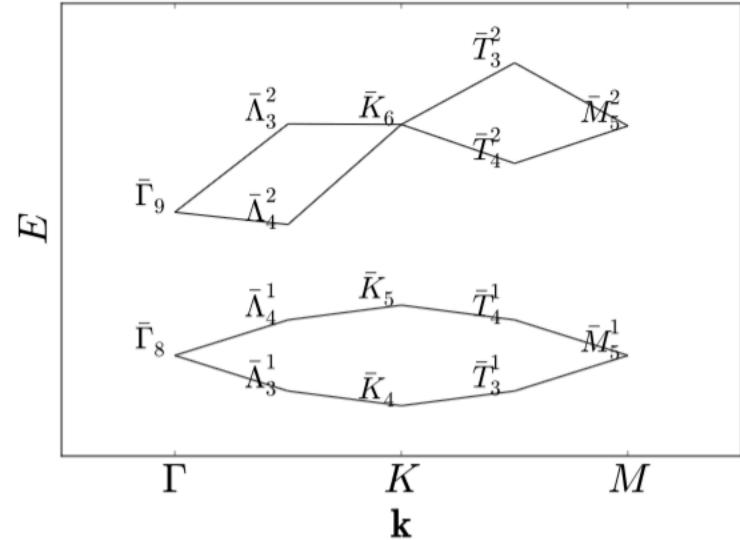
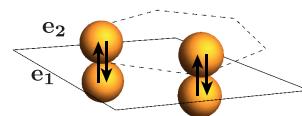
Example: Graphene



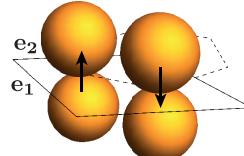
Example: Graphene



(a)
Connected EBR



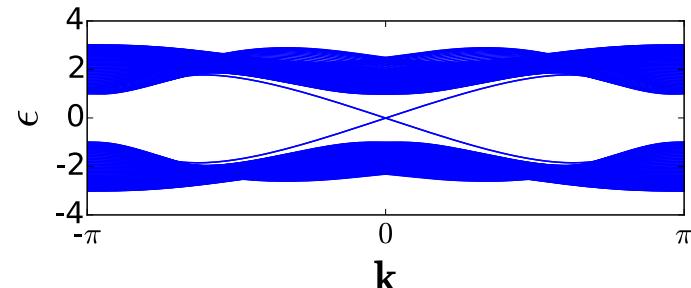
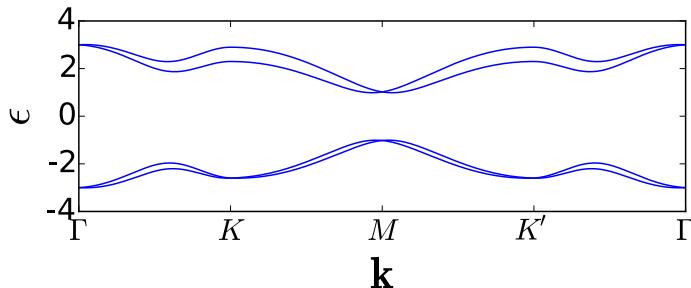
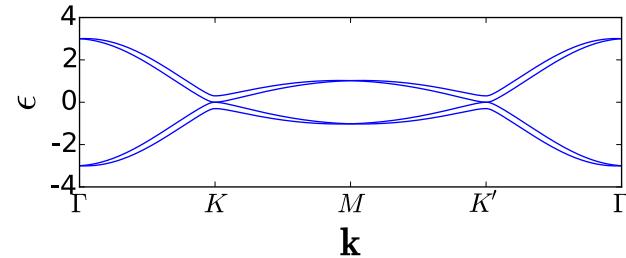
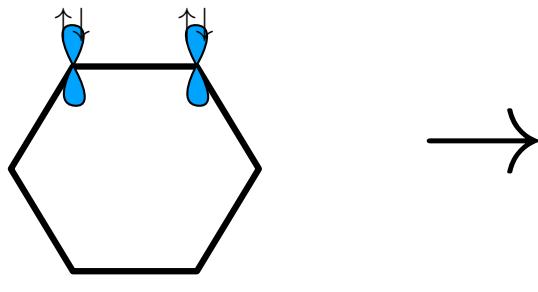
(b)
Disconnected EBR



Topological insulator

Split pEBR

- Elementary Band representations that also respect time-reversal symmetry in real space are physical band representations (pEBRs).



EBRs in TQC

- Band reps coming from irreps of **maximal** G_q are connected in trivial phases.
- Elementary Building blocks for **all atomic-limit** band structures. There are 10,403 (with/without time reversal: 4,757/5,646) EBRs in total for all 230 space groups, listed on the Bilbao Crystallographic Server (<http://www.cryst.ehu.es/cgi-bin/crst/programs/bandrep.pl>)
- Main result: Any isolated set of bands that is not equivalent to a sum of elementary band representations gives a topological (crystalline) insulator.

Outline

- Brief introduction to topological states
- Topological Quantum Chemistry (TQC)
- Applications in materials search

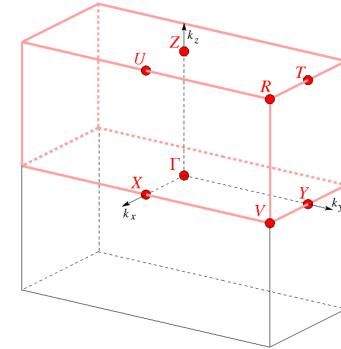
Applications in materials search

- Compute the eigenstates at **several** k-points (< 10).
- Get the irreps from the eigenstates.
- Solve the compatibility relations: semimetal or insulator.
- Insulator: If it's can be decomposed into a sum of EBRs
(Yes: Trivial No: Topological)

Application in SG 2

<http://www.cryst.ehu.es/cgi-bin/cryst/programs/bandrep.pl>

Wyckoff pos.	1a($\bar{1}$)	1a($\bar{1}$)	1b($\bar{1}$)	1b($\bar{1}$)	1c($\bar{1}$)	1c($\bar{1}$)	1d($\bar{1}$)	1d($\bar{1}$)
Band-Rep.	$A_g \uparrow G(1)$	$A_u \uparrow G(1)$	$A_g \uparrow G(1)$	$A_u \uparrow G(1)$	$A_g \uparrow G(1)$	$A_u \uparrow G(1)$	$A_g \uparrow G(1)$	$A_u \uparrow G(1)$
Decomposable Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable
$\Gamma:(0,0,0)$	$\Gamma_1^+(1)$	$\Gamma_1^-(1)$	$\Gamma_1^+(1)$	$\Gamma_1^-(1)$	$\Gamma_1^+(1)$	$\Gamma_1^-(1)$	$\Gamma_1^+(1)$	$\Gamma_1^-(1)$
$R:(1/2,1/2,1/2)$	$R_1^+(1)$	$R_1^-(1)$	$R_1^-(1)$	$R_1^+(1)$	$R_1^-(1)$	$R_1^+(1)$	$R_1^-(1)$	$R_1^+(1)$
$T:(0,1/2,1/2)$	TRIM							
$U:(1/2,0,1/2)$	$\Gamma \ X \ Y \ Z \ S \ T \ U \ R$							
$V:(1/2,1/2,0)$	No. of $\lambda_I = -1$							
$X:(1/2,0,0)$	12	14	14	14	14	14	14	14
$Y:(0,1/2,0)$	TABLE I: The number of Kramers pairs with -1 parity eigenvalues at each of the TRIM points in β -MoTe ₂ , obtained from							
$Z:(0,0,1/2)$								

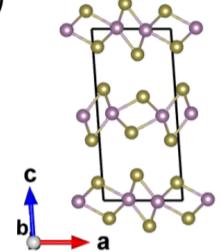


- The total number of (pairs of) odd/even parity bands at all TRIM points is a multiple of 4.
- The total number of (pairs of) odd/even parity bands for any TRIM plane is a multiple of 2.

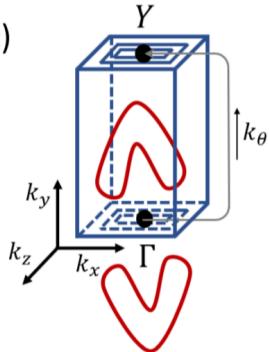
MoTe₂

<https://arxiv.org/abs/1806.11116>

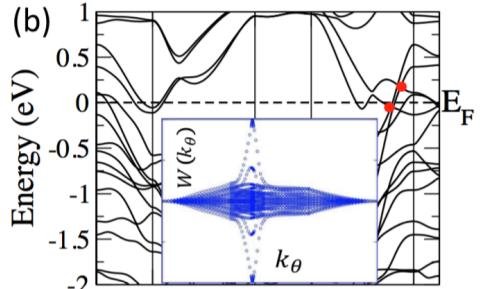
(a)



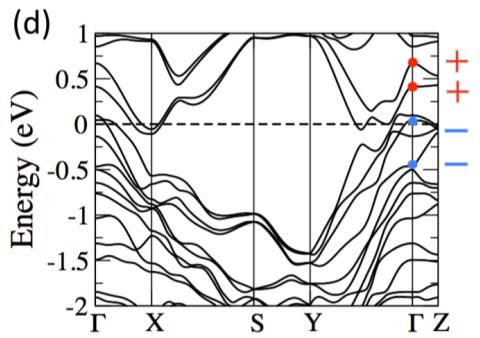
(c)



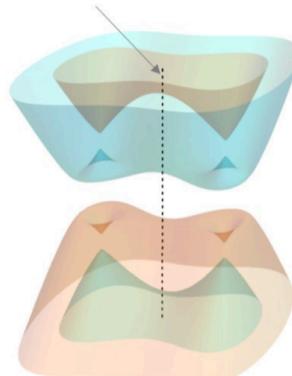
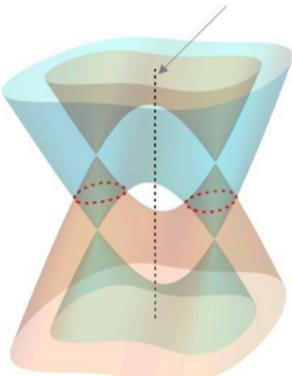
(b)



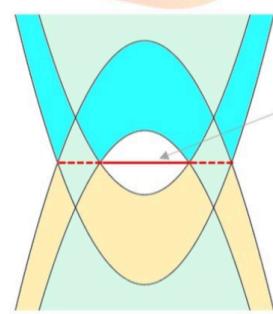
(d)



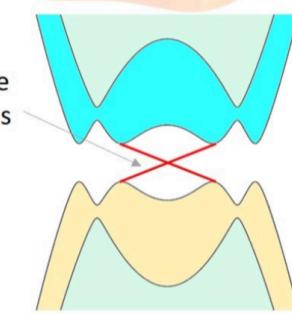
double band inversion



topological nodal line
semimetal
(without SOC)



higher order
topological insulator
(with SOC)



Application in Bi

- Completely trivial

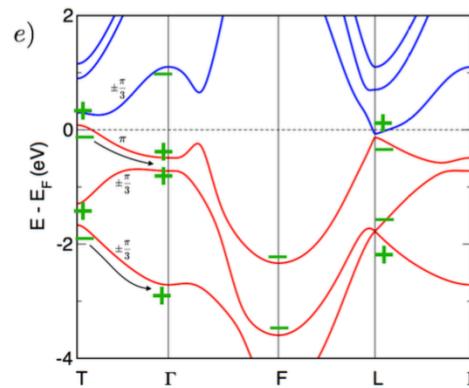
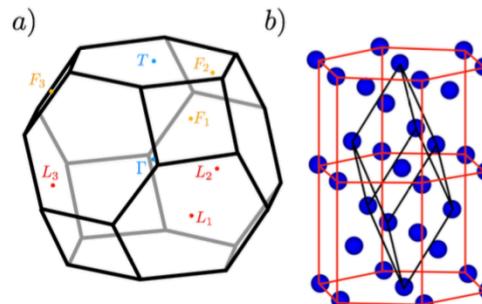
$$\Gamma (0 \ 0 \ 0)$$

$$T (\pi, \pi, \pi)$$

$$F (\pi, \pi, 0)$$

$$L (\pi, 0, 0)$$

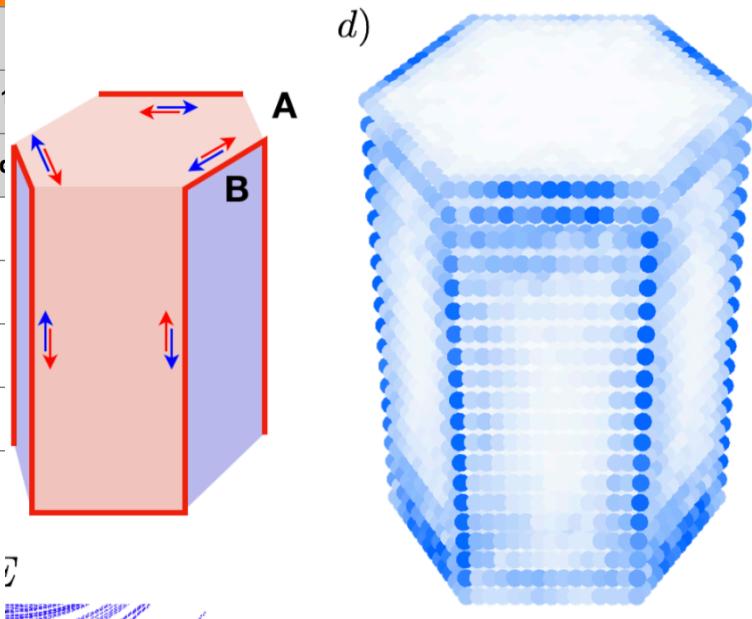
Bi	
1Γ	$+, -, +, +, +; (-)$
$3L$	$+, -, +, -, -; (-)$
$3X$	$-, +, +, -, -; (-)$
T	$-, +, -, +, -; (-)$
Z_2	$(0;000)$



EBR analysis

Wyckoff pos.	3a($\bar{3}m$)	3a($\bar{3}m$)	3a($\bar{3}m$)	3a($\bar{3}m$)	
Band-Rep.	$^1\bar{E}_g \ 2\bar{E}_g \uparrow G(2)$	$^1\bar{E}_u \ 2\bar{E}_u \uparrow G(2)$	$\bar{E}_{1g} \uparrow G(2)$	$\bar{E}_{1u} \uparrow G(2)$	
Decomposable Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable
$\Gamma:(0,0,0)$	$\bar{\Gamma}_4 \bar{\Gamma}_5(2)$	$\bar{\Gamma}_6 \bar{\Gamma}_7(2)$	$\bar{\Gamma}_8(2)$	$\bar{\Gamma}_9(2)$	
$T:(0,0,3/2)$	$\bar{T}_4 \bar{T}_5(2)$	$\bar{T}_6 \bar{T}_7(2)$	$\bar{T}_8(2)$	$\bar{T}_9(2)$	
$F:(0,1/2,1)$	$\bar{F}_3 \bar{F}_4(2)$	$\bar{F}_5 \bar{F}_6(2)$	$\bar{F}_3 \bar{F}_4(2)$	$\bar{F}_5 \bar{F}_6(2)$	
$L:(-1/2,1/2,1/2)$	$\bar{L}_3 \bar{L}_4(2)$	$\bar{L}_5 \bar{L}_6(2)$	$\bar{L}_3 \bar{L}_4(2)$	$\bar{L}_5 \bar{L}_6(2)$	

	3 doubly-degenerate valence bands
F	$F_3 F_4; \bar{F}_5 \bar{F}_6; \bar{F}_5 \bar{F}_6$
Γ	$\bar{\Gamma}_8; \bar{\Gamma}_8; \bar{\Gamma}_4 \bar{\Gamma}_5$
L	$\bar{L}_3 \bar{L}_4; \bar{L}_5 \bar{L}_6; \bar{L}_5 \bar{L}_6$
T	$\bar{T}_9; \bar{T}_8; \bar{T}_6 \bar{T}_7$



<https://arxiv.org/abs/1802.02585>

High through-put search in ICSD

ARTICLE

<https://doi.org/10.1038/s41586-019-0954-4>

A complete catalogue of high-quality topological materials

M. G. Vergniory^{1,2,3,11}, L. Elcoro^{4,11}, Claudia Felser⁵, Nicolas Regnault⁶, B. Andrei Bernevig^{7,8,9*} & Zhijun Wang^{7,10*}

We provide an open-source code that checks the topology of any material and allows other researchers to reproduce our results.

results show that more than 27 per cent of all materials in nature are topological. We provide an open-source code that checks the topology of any material and allows other researchers to reproduce our results.

Similar works

- Barry Bradlyn et al., "Topological quantum chemistry", Nature, 547 (2017).
 - a. Irrep tables for all k points for all the space groups.
 - b. Compatibility relations.
 - c. List of all the EBRs.
- Po, H. C. et al., "Symmetry-based indicators of band topology in the 230 space groups", Nat. Comm. 8, 50 (2017)
 - a. Classification.
- Z. Song et al., "Quantitative mappings between symmetry and topology in solids", Nat. Comm. 9, 3530 (2018)
 - a. Symmetry indicators
 - b. **the full list of TCI.**

	Barary2017	PoHC2017
Irreps	✓	x
Comp.	✓	x
EBR (AI)	✓	x
Class.	x	✓

the indicator group $\{\text{BS}\}/\{\text{AI}\}$ is $\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_4$

$$z_{2,1} \equiv \sum_{\substack{\mathbf{K} \in \text{TRIM} \\ \text{at } \{k_1=\pi\}}} \frac{N_-(\mathbf{K}) - N_+(\mathbf{K})}{2} \bmod 2$$

$$z_{2,2} \equiv \sum_{\substack{\mathbf{K} \in \text{TRIM} \\ \text{at } \{k_2=\pi\}}} \frac{N_-(\mathbf{K}) - N_+(\mathbf{K})}{2} \bmod 2$$

$$z_{2,3} \equiv \sum_{\substack{\mathbf{K} \in \text{TRIM} \\ \text{at } \{k_3=\pi\}}} \frac{N_-(\mathbf{K}) - N_+(\mathbf{K})}{2} \bmod 2$$

$$z_4 \equiv \sum_{\mathbf{K} \in \text{TRIM}} \frac{N_-(\mathbf{K}) - N_+(\mathbf{K})}{2} \bmod 4$$

Similar results

- Irreps in high-symmetry points – same results.
- Tang, F., et al., “Comprehensive search for topological materials using symmetry indicators”, Nature 566, 486-489 (2019) – Atomic Insulators.
- Zhang, T., et al., “Catalogue of topological electronic materials”, Nature 566, 475-479 (2019) – symmetric indicators.
- Vergniory, M.G., et al., “A complete catalogue of high-quality topological materials”, Nature, 566, 480-485 (2019). – EBR(TQC)

Check any material by yourself

The open-source code VASP2Trace and end-user button CheckTopologicalMat are available online at
<http://www.cryst.ehu.es/cryst/checktopologicalmat>.

1. Obtain the eigenstates at several k-points. (VASP)
2. Compute the irreps from the eigenstates. (“irvsp”, “vasp2trace”)
 - a. Download “vasp2trace” : www.cryst.ehu.es/cryst/checktopologicalmat, which includes a folder of “max_KPOINTS_VASP/” and a source code of “src_trace_v1.tar.gz”
 - b. Install “vasp2trace” with the source: vasp2trace/src_trace_v1.tar.gz
3. Solve the compatibility relations: semimetal or **Insulator**. (“checktopologicalmat”).
Insulator: check If it's can be decomposed into a sum of EBRs.
(Yes: Trivial No: **Topological**)
Topological: Compute the symmetry indicators

Ref: Vergniory, M.G., et al., “A complete catalogue of high-quality topological materials”, Nature, 566, 480-485 (2019)

www.cryst.ehu.es/cryst/checktopologicalmat

Check Topological Mat

Check Topological Mat.

Given a file that contain the eigenvalues at each maximal k-vec of a space group, the program gives the set of irreducible representations at each maximal k-vec (time-reversal is assumed). Then, using the compatibility relations and the set of Elementary Band Representations (EBRs), it checks whether the set of bands can be put as linear combinations of EBRs. This (self-explanatory) file shows the format of the file to be uploaded in the menu on the right:

File_Description

You can download examples of input files here:

[Example_Ag1Ge1Li2](#)

[Example_B2Ca3Ni7](#)

[Example_Ba3Ca1O9Pu2](#)

[Example_Ag1O2Sc1](#)

[Example_of_Bad_File](#)

You can generate the "trace.txt" file in your own computer using VASP and this program (fortran).

[vasp2trace](#)

Read the "README.pdf" file for help on the use of vasp2trace.

If you are using "Check Topological Mat." and/or "vasp2trace" programs in the preparation of an article, please cite this reference:

M.G. Vergniory, L. Elcoro, C. Felser, N. Regnault, B.A. Bernevig, Z. Wang

Nature(2019) **566**, 480-485. doi:10.1038/s41586-019-0954-4

Upload your traces.txt file (see the help in the column on the left).

Show

Ex: Bi₂Se₃

- 1. The SG number(166) and crystal structure.
(run “Phonopy” to make sure the POSCAR is given in a standard setting.)
- 2. Get the high-symmetry k points for that SG (166).
(Vasp2trace/max_KPOINTS_VASP_KPOINTS_166.txt).
- 3. Run “VASP”, to obtain the eigen-states(WAVECAR) at those kpoints.
(check the symmetry operators in OUTCAR, simply by counting the total number of the operators)
- 4. Run “vasp2trace” that you have just installed locally in the folder.
(trace.txt would be generated automatically)
- 5. Upload “trace.txt” and press the button.

Step 1:

```
$ phonopy --tolerance 0.01 --symmetry -c POSCAR  
$ vim PPOSCAR  
$ cp PPOSCAR POSCAR
```

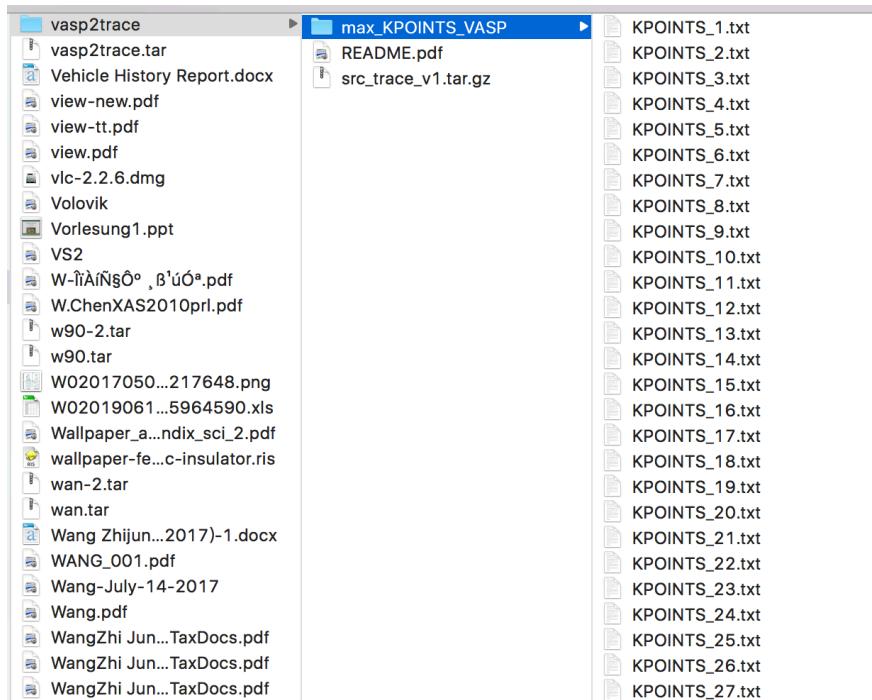
```
/anaconda3/bin/phonopy --tolerance 0.01 --symmetry -c POSCAR  
phonopy_version: '1.13.2'  
space_group_type: 'R-3m'  
space_group_number: 166  
point_group_type: '-3m'  
space_group_operations:  
- rotation: # 1  
- [ 1, 0 , 0]  
- [ 0, 1 , 0]  
- [ 0, 0 , 1]  
translation: [ 0.00000, 0.00000, 0.00000 ]  
- rotation: # 2  
- [-1, 0 , 0]  
- [ 0, -1 , 0]  
- [ 0, 0 ,-1]  
translation: [ 0.00000, 0.00000, 0.00000 ]
```

“POSCAR”

```
1 generated by phonopy  
2 1.0  
3 2.0690000000000000 1.1945377069533354 9.5466666571200012  
4 -2.0690000000000000 1.1945377069533354 9.5466666571200012  
5 0.0000000000000000 -2.3890754139066708 9.5466666571200012  
6 Bi Se  
7 2 3  
8 Direct  
9 0.6009999996010008 0.6009999996010008 0.6009999996010009  
10 0.3990000003989990 0.3990000003989991 0.3990000003989989  
11 0.7939999997940036 0.7939999997940036 0.7939999997940036  
12 0.2060000002059964 0.2060000002059964 0.2060000002059964  
13 0.0000000000000000 0.0000000000000000 0.0000000000000000  
-  
"PPOSCAR" 13L, 560C
```

Step 2:

```
$ cp xx/vasp2trace/max_KPOINTS_VASP/KPOINTS_166.txt KPOINTS.high
```



Step 3:

Follow README in the folder VASP2trace

- a. Run the scf calcualtion in vasp
- b. Run the band calculation in vasp with KPOINTS.high

```
$ vim OUTCAR; ./irot
```

```
399 Automatic generation of k-mesh.  
400 Space group operators:  
401 irot      det(A)      alpha      n_x      n_y      n_z      tau_x      tau_y      tau_z  
402   1      1.000000      0.000000      1.000000      0.000000      0.000000      0.000000      0.000000      0.000000  
403   2     -1.000000      0.000000      1.000000      0.000000      0.000000      0.000000      0.000000      0.000000  
404   3      1.000000    180.000000      0.866025      0.500000      0.000000      0.000000      0.000000      0.000000  
405   4     -1.000000    180.000000      0.866025      0.500000      0.000000      0.000000      0.000000      0.000000  
406   5      1.000000    120.000000      0.000000      0.000000      -1.000000      0.000000      0.000000      0.000000  
407   6     -1.000000    120.000000      0.000000      0.000000      -1.000000      0.000000      0.000000      0.000000  
408   7      1.000000  179.999999      0.000000      1.000000      0.000000      0.000000      0.000000      0.000000  
409   8     -1.000000  179.999999      0.000000      1.000000      0.000000      0.000000      0.000000      0.000000  
410   9      1.000000    120.000000      0.000000      0.000000      1.000000      0.000000      0.000000      0.000000  
411  10     -1.000000    120.000000      0.000000      0.000000      1.000000      0.000000      0.000000      0.000000  
412  11      1.000000    180.000000      0.866025     -0.500000      0.000000      0.000000      0.000000      0.000000  
413  12     -1.000000    180.000000      0.866025     -0.500000      0.000000      0.000000      0.000000      0.000000  
414  
415 Subroutine IBZKPT returns following result:
```

Step 4:

```
$ vasp2trace / vasp2trace $nele
```

```
1 28
2 1
3 12
4 1 0 0 0 1 0 0 0 1 0.000000 0.000000 0.000000 1.000000 0.000000 0.000000 0.000000 0.000000
5 -1 0 0 0 -1 0 0 0 -1 0.000000 0.000000 0.000000 1.000000 0.000000 0.000000 0.000000 0.000000
6 -1 0 0 0 0 -1 0 -1 0 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.500000 0.8660
7 1 0 0 0 0 1 0 1 0 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.500000 0.8660
8 0 0 1 1 0 0 0 1 0 0.000000 0.000000 0.000000 0.500000 -0.866025 0.000000 0.000000 0.000000
9 0 0 -1 -1 0 0 0 -1 0 0.000000 0.000000 0.000000 0.500000 -0.866025 0.000000 0.000000 0.000000
10 0 -1 0 -1 0 0 0 0 -1 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 1.000000 0.000000
11 0 1 0 1 0 0 0 0 1 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 1.000000 0.000000
12 0 1 0 0 0 1 1 0 0 0.000000 0.000000 0.000000 0.500000 0.866025 0.000000 0.000000 0.000000
13 0 -1 0 0 0 -1 -1 0 0 0.000000 0.000000 0.000000 0.500000 0.866025 0.000000 0.000000 0.000000
14 0 0 -1 0 -1 0 -1 0 0 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 -0.500000 0.8660
15 0 0 1 0 1 0 1 0 0 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 -0.500000 0.8660
16 4
17 0.000000 0.000000 0.000000
18 0.500000 0.500000 0.500000
19 0.500000 0.500000 0.000000
20 0.000000 0.500000 0.000000
21 12
22 1 2 -9.773922 2.000000 0.000000 2.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.0
23 1 2 -8.564873 2.000000 0.000000 -2.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.0
24 3 2
```

Step 5:

topological Mat

Upload your traces.txt file (see the help in the column on the left)

选取文件 trace.txt
Show

Result of the analysis of the uploaded structure

- The material is a topological insulator.
- List of topological indices:
 $z_{2w,1}=0$
 $z_{2w,2}=0$
 $z_{2w,3}=0$
 $z_4=3$
- The material belongs to the strong topological class: 6
- Clicking on [See the irreps](#) you can see the details about the number of bands and the identified irreps at each maximal k-vector.
- The set of bands can be put as linear combination of Elementary Band Representations (EBR) and parts of decomposable EBRs with integer positive coefficients. Click on [Linear Combinations](#) to get some possible linear combinations of EBRs and partial EBRs.
- Click on [Subgroups](#) to check the topological character of the structure in each of its (translationengleiche) subgroups.

Take-home message

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Topological: Compute the symmetry indicators

Ref: Vergniory, M.G., et al., “A complete catalogue of high-quality topological materials”, Nature, 566, 480-485 (2019)

欢迎各位学生学者联系我们，来本组学习访问。欢迎博士后加入！！

Contact us via email : wzj@iphy.ac.cn or zjwang11@hotmail.com

Thanks for your attention!